

The Overlap Dirac Operator [★]

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Abstract. This introductory presentation describes the Overlap Dirac Operator, why it could be useful in numerical QCD, and how it can be implemented.

1 Introduction

The objective of this talk is to introduce a certain matrix, the Overlap Dirac Operator. The ideas behind this construction are rather deep, having to do with the self-consistency of chiral gauge theories [1]. Chiral gauge theories are a class of quantum field theoretical models from which one draws the minimal standard model of particle physics. This model describes all phenomena at distances larger than about 10^{-18} meters, excluding gravity.

The Overlap Dirac Operator may be useful also in numerical studies of the strong interaction component of the minimal standard model, Quantum Chromo-Dynamics (QCD). QCD, in isolation, is a vector-like gauge theory, a simple combination of chiral gauge theories within which some of the mathematical complexities of the general class disappear. Nevertheless, the strong nonlinearity of QCD makes the quantitative evaluation of its most basic observable features possible only within large scale numerical Monte Carlo simulations. This workshop will deal mainly with numerical QCD, the subfield of lattice field theory which focuses on such simulations.

Therefore, the form of the Overlap Dirac Operator will be motivated heuristically, based on technical considerations of numerical QCD. The heuristic motivation will start from the continuum Euclidean Dirac operator, whose basic features of direct relevance to numerics will be reviewed. As alluded above, this is not the original way the Overlap Dirac Operator was found, but, for the focus of this workshop it is unnecessary to go through the entire construction. Rather, I shall start by reviewing an important technicality, the light quark bottleneck, which is a serious problem in contemporary traditional numerical QCD, argue that there is no fundamental reason why this bottleneck cannot be avoided and present the Overlap Dirac Operator

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as a potential solution¹. The solution is not yet working efficiently because another bottleneck appears. However, the new bottleneck may be easier to circumvent than the old one.

An effort has been made to make this presentation accessible to applied mathematicians. Physicists practicing numerical QCD, in particular when the Overlap Dirac Operator is used, are facing issues that the expertise of specialists in numerical linear algebra could be of great help in resolving. These same physicists will likely be familiar with large portions of the presentation below, perhaps excepting the way the Overlap Dirac Operator is arrived at.

2 The numerical bottleneck of light quarks

The QCD Lagrangian with correct parameters should produce the observed ratio of masses $\frac{m_\pi}{m_\rho} = 0.18$. The relative smallness of this number reflects the relative small mass of two of the lightest quarks in Nature. This mass is not only small relatively to other quark masses, but, more importantly, relative to a basic scale of QCD itself, a mass parameter known as Λ_{QCD} . Theoretically, one has very good reasons to expect to be able to smoothly extrapolate in the light quark masses from, say, $\frac{m_\pi}{m_\rho} = 0.25$ to the smaller physical value. Actually, even the functional form of these extrapolations is known. However, it is not likely that the extrapolation will go smoothly through the value $\frac{m_\pi}{m_\rho} = 0.5$. As long as $\frac{m_\pi}{m_\rho} \geq 0.5$ the decay $\rho \rightarrow 2\pi$ is energetically forbidden but once this threshold is passed the decay becomes allowed. This provides physical reasons to expect a “bumpy” behavior² in the extrapolation to light quark masses in the region where $\frac{m_\pi}{m_\rho} \sim 0.5$ and there are no first principle based theoretical expressions parameterizing this “bumpy” region. Current large scale numerical work happens to be close to the threshold $\frac{m_\pi}{m_\rho} = 0.5$, and there are numerical difficulties obstructing straightforward attempts to go significantly lower.

¹ Other solutions than the Overlap Dirac Operator have been proposed for this specific problem; using the Overlap Dirac Operator is probably the most fundamentally motivated approach, but the cost may be high, and at the bottom line this consideration often takes precedence.

² Some quantities may be insensitive to the $\rho \rightarrow 2\pi$ threshold effects, typically for kinematic reasons. Also, there is an additional approximation which is very often employed (the so called “valence”, or “quenched” approximation) which eliminates decay effects on the vacuum of the theory. On the other hand, one often relies on an effective low energy description of QCD, in which the Lagrangian is replaced by an “effective Lagrangian” involving only π ’s and some other light associated particles. The existence of a particle like the ρ and its connection to the 2π state is then encoded in the coefficients of the “effective Lagrangian” and will affect the accuracy of chiral perturbation theory at moderate energies. Thus, physical observables related to “weak matrix elements” are an example where one might suspect sensitivity to threshold effects.

In numerical work one uses a lattice whose spacing a is measured in inverse mass units. Thus any number of the type $\text{mass} \times a$ is a pure number, of the kind a computer can handle. The threshold ratio is obtained, with current simulation parameters, for $m_\pi a \sim 0.1$ and for quark mass m_q given by $m_q a \sim 0.05$. Nothing is lost by setting $a = 1$; dimensional considerations can always restore the right power of a . Physical considerations imply $m_\pi \propto \sqrt{m_q}$ for small m_q . On the other hand, m_ρ stays finite (basically of the order of Λ_{QCD}) at $m_q = 0$ and consequently its numerical dependence on m_q for small m_q is weaker. So, in order to reduce $\frac{m_\pi}{m_\rho}$ by a factor of 2 as we would like, we have to reduce the light quark masses by about a factor of 4. The bottom line is that we would like to leave all other simulation parameters the same, only change the quark mass to something like $m_q a = 0.01$.

Simple arguments indicate that we should be able to do that. The quark mass enters as an important parameter in the lattice Dirac Operator, D . D and $D^\dagger D$ are matrices that need to be inverted on vectors in the most inner procedure of the simulations. In traditional simulations D is a sparse matrix; full storage is out of the question, as the dimension of D is too large. The quark mass directly affects the condition number of D , so its value can easily become the bottleneck of the entire simulation. But, we could easily imagine being lucky enough to manage the needed value of $m_q a = 0.01$: D is a discretized first order partial differential operator and, since space time is four dimensional one can easily think of D obeying $\|D\| \leq 4$ as a uniform upper bound. On the other hand, m_q enters additively, with unit coefficient and, based on the continuum formula one would expect that D is approximately anti-hermitian at zero quark mass. Therefore, we expect $\|D^\dagger D\| \geq m_q^2$ and, when we invert $D^\dagger D$, a condition number of the order 10^5 , which should allow the evaluation of $\frac{1}{D^\dagger D} \psi$ in something like 500-1000 iterations.

Up to relatively short lived jerks, computational power is projected to increase by Moore's Law for another decade, so we can expect an enhancement by a factor of 250 at fixed power dissipation by 2010. Based on the accumulated numerical experience to date, we can reasonably expect that, by then, we would be able to carry out our computations with relative ease.

However, the sad fact is that theoretical issues have apparently made it impossible to find a simple enough D which would obey the rather plausible lower bound $\|D^\dagger D\| \geq m_q^2$. This was a key assumption I made before in order to come up with the condition number of order 10^5 . What really happens in the traditional approach³ is that $D^\dagger + D$ is not small and to get $\frac{m_\pi}{m_\rho} \sim .3$ one is forced into a regime where the lowest eigenvalue of $D^\dagger D$ quite often fluctuates as low as 10^{-8} . This makes the condition number go to 10^{10} and puts the $\frac{m_\pi}{m_\rho} \sim .3$ mass ratio out of numerical reach.

The above numerical problem reflects a difficulty of principle associated with the $m_q = 0$, or massless, case. In the continuum model, $m_q = 0$ is

³ To be specific, the approach employing Wilson fermions; there also exists a traditional "staggered fermion" alternative, but it suffers from other problems.

associated with an extra symmetry, chirality. Technically, chirality ensures that in the continuum the massive Dirac operator $D + m_q$ (where I reserved D for the massless case) indeed obeys $\|D^\dagger D\| \geq m_q^2$. But, chirality cannot be preserved on the lattice in the same way as some other symmetries can. For twenty years it was thought that an acceptable lattice version of D which also preserves chirality does not exist. The good news is that a series of developments, started in 92 by Kaplan and by Frolov and Slavnov [2] and built on by Narayanan and myself, have produced, in 97, the Overlap Dirac Operator D_o on the lattice, which, effectively has the extra symmetry. While D_o is easy to write down, it is not easy to implement because it no longer is sparse. There nevertheless is some hope, because, in the most common implementation of the Overlap ideas, D_o is what probably would be the next best thing: up to trivially implemented factors, it is a function (as an operator) of a sparse matrix⁴. Unfortunately, the function has a discontinuity, so its implementation is costly. The numerical developments in this subfield are relatively fresh and substantial progress has been achieved but we are not yet adequately tooled for full “production runs”. Still, since the time we have had to address the problem is of the order of a year or two I think further substantial progress is likely.

3 Dirac Operator basics

The Dirac Operator is a very important object in relativistic Field Theory. Among other things, it predicted the existence of the electron anti-particle, the positron. All of known matter is governed by the Dirac equation.

3.1 Continuum

The Dirac Operator is defined in the continuum (Euclidean space) by

$$D_c = \sum_{\mu} \gamma_{\mu} (\partial_{\mu} + iA_{\mu}) , \quad (1)$$

where,

$$\gamma_{\mu}^{\dagger} = \gamma_{\mu}; \quad \mu = 1, 2, 3, 4; \quad \{\gamma_{\mu}, \gamma_{\nu}\} \equiv \gamma_{\mu}\gamma_{\nu} + \gamma_{\nu}\gamma_{\mu} = 2\delta_{\mu\nu} . \quad (2)$$

We also have,

$$A_{\mu} = A_{\mu}^{\dagger}; \quad \text{tr} A_{\mu} = 0; \quad A_{\mu} \text{ are } 3 \text{ by } 3 \text{ matrices.} \quad (3)$$

The notation ∂_{μ} indicates $\partial/\partial x_{\mu}$. A_{μ} is x -dependent, but the γ_{μ} are constant four by four matrices and operate in a separate space. Thus, D_c is a twelve

⁴ The additional “trivial” factors have a highly non-trivial numerical impact: because of them the *inverse* of D_o no longer has a simple expression in terms of a function of a sparse matrix.

by twelve matrix whose entries are first order partial differential operators on a four dimensional Euclidean space, henceforth assumed to be a flat four torus. The massive Dirac Operator is $m_c + D_c$.

The main properties of the Dirac Operator are:

1. For $A_\mu = 0$ one can set by Fourier transform $\partial_\mu = ip_\mu$ giving $D_c = i\gamma_\mu p_\mu$. This produces $D_c^2 = -\sum_\mu p_\mu^2$ from the algebra of the γ -matrices. The important consequence this has is that $D_c = 0$ iff $p_\mu = 0$ for all μ .
2. Define $\gamma_5 \equiv \gamma_1\gamma_2\gamma_3\gamma_4$ which implies $\gamma_5^2 = 1$ and $\gamma_5\gamma_\mu + \gamma_\mu\gamma_5 = 0$. The property of γ_5 -hermiticity is that D_c is hermitian under an indefinite inner product defined by γ_5 , or, equivalently, using the standard L_2 inner product, we have for any backgrounds A_μ and any mass parameter m_c

$$\gamma_5(D_c + m_c)\gamma_5 = (D_c + m_c)^\dagger . \quad (4)$$

Thus, γ_5 -hermiticity is a property of the massive Dirac Operator.

3. At zero mass the Dirac Operator is anti-hermitian $D_c^\dagger = -D_c$. This property, in conjunction with γ_5 -hermiticity implies the symmetry property of chirality: $\gamma_5 D_c \gamma_5 = -D_c$ usually written as $\{D_c, \gamma_5\} = 0$. Traditionally, anti-hermiticity would be viewed as a separate and trivial property and chirality as a symmetry. Then, γ_5 hermiticity would be a consequence holding not only for the massless Dirac Operator, but also for non-zero mass. But, for better comparison to the lattice situation it is somewhat better to exchange cause and consequence, as done here.

3.2 Lattice

Numerical QCD spends most of the machine cycles inverting a lattice version of the massive Dirac Operator. This is how the continuum Dirac operator is discretized:

The continuum x is replaced by a discrete lattice site x on a torus. The matrix valued functions A_μ are replaced by unitary matrices $U_\mu(x)$ of unit determinant. $U_\mu(x)$ is associated with the link l going from x into the positive μ -direction, $\hat{\mu}$.

The connection to the continuum is as follows: Assume that the functions⁵ $A_\mu(x)$ are given. Then,

$$\begin{aligned} U_\mu &= \lim_{N \rightarrow \infty} [e^{iaA_\mu(x)/N} e^{iaA_\mu(x+a)/N} e^{iaA_\mu(x+2a)/N} \dots e^{iaA_\mu(x+(N-1)a)/N}] \\ &\equiv P \exp[i \int_l dx_\mu A_\mu(x)] \quad (\text{the symbol P denotes "path ordering"}) . \end{aligned} \quad (5)$$

There are two sets of basic unitaries acting on twelve component vectors $\psi(x)$:

⁵ Actually, the $A_\mu(x)$ aren't really functions, rather they make up a one form $\sum_\mu A_\mu(x) dx_\mu$ which is a connection on a possibly nontrivial bundle with structure group $SU(3)$ over the four-torus. This complication is important for the case of massless quarks, but shall be mostly ignored in the following.

1. The point wise acting γ_μ 's and
2. the directional parallel transporters T_μ , defined by:

$$T_\mu(\psi)(x) = U_\mu(x)\psi(x + \hat{\mu}) . \quad (6)$$

There also is a third class of unitaries carrying out gauge transformations. Gauge transformations are characterized by a collection of $g(x) \in SU(3)$ and act on ψ pointwise. The action is represented by the unitary $G(g)$, so that $(G(g)\psi)(x) = g(x)\psi(x)$. Probably the most important property of the T_μ operators is that they are “gauge covariant”,

$$G(g)T_\mu(U)G^\dagger(g) = T_\mu(U^g) , \quad (7)$$

where,

$$U_\mu^g(x) = g(x)U_\mu(x)g^\dagger(x + \hat{\mu}) . \quad (8)$$

The variables $U_\mu(x)$ are stochastic, distributed according to a probability density that is invariant under $U \rightarrow U^g$ for any g .

The lattice replacement of the massive continuum Dirac Operator, $D(m)$, is an element in the algebra generated by T_μ , T_μ^\dagger , γ_μ . Thus, $D(m)$ is gauge covariant. For $U_\mu(x) = 1$ the T_μ become commuting shift operators. One can preserve several crucial properties of the continuum Dirac Operator by choosing a $D(m)$ which satisfies:

1. Hypercubic symmetry. This discrete symmetry group consists of 24 permutations scrambling the μ indices (which leave $D(m)$ unchanged) combined with 16 reflections made out of the following four elementary operations:

$$\gamma_5 \gamma_\mu D(T_\mu \longleftrightarrow T_\mu^\dagger)(m) \gamma_\mu \gamma_5 = D(m) . \quad (9)$$

2. Correct low momentum dependence. When the commutators $[T_\mu, T_\nu] = 0$ one can simultaneously diagonalize the T_μ unitaries, with eigenvalues $e^{i\theta_\mu^k}$. For small θ angles, one gets $D(m) \sim m + i \sum_\mu \gamma_\mu \theta_\mu + O(\theta^2)$. One also needs to require that for zero mass ($m = 0$) $D^\dagger D$ be bounded away from zero for all θ which are outside a neighborhood R of zero.
3. Locality and smoothness in the gauge field variables. One can also require, at least for gauge backgrounds with small enough (in norm) commutators $[T_\mu, T_\nu]$, that D be a convergent series in the T_μ .

The simplest solution to the above requirements is the Wilson Dirac Operator, D_W . It is the sparsest possible realization of the above. Fixing a particular free parameter (usually denoted by r) to its preferred value ($r = 1$) D_W can be written as:

$$D_W = m + 4 - \sum_\mu V_\mu; \quad V_\mu^\dagger V_\mu = 1; \quad V_\mu = \frac{1 - \gamma_\mu}{2} T_\mu + \frac{1 + \gamma_\mu}{2} T_\mu^\dagger . \quad (10)$$

For $m > 0$ clearly $\|D_W\| \geq m$, but to get the physical quark mass to zero, $m_q^{\text{phys}} = 0$, one needs to take into account an additive renormalization induced by the fluctuations in the gauge background $U_\mu(x)$: m must be chosen as $m = m_c(\beta) < 0$ where β is the lattice version of the gauge coupling constant governing the fluctuations of the background. The need to use a negative m on the lattice opens the door for very small eigenvalues for $D_W^\dagger D_W$ and thus for terrible condition numbers. To get a small but nonzero physical quark mass one should choose $m = m_c(\beta) + \Delta m$, $\Delta m > 0$ but the numbers are such that one always ends up with an overall negative m .

3.3 A simplified “no-go theorem”.

These problems would go away if we had chirality, because it would single out the $m = 0$ values as special and remove the additive renormalization. But, this cannot be done. There are rather deep reasons for why this cannot be done, and several versions of “no-go theorems” exist[3]. Here, I shall present only a very simple version, namely, one cannot supplement the above requirements of $D(m)$ (fulfilled by D_W) with the requirement $\gamma_5 \tilde{D} \gamma_5 = -\tilde{D}$ at $m = 0$. The proof is very simple: Take the particular case where the T_μ commute. Compounding four elementary reflections we get $\gamma_5 \tilde{D}(\theta) \gamma_5 = \tilde{D}(-\theta) = -\tilde{D}(\theta)$. This shows that any one of the sixteen solutions $\theta_\mu = 0, \pi$ has $\tilde{D}(\theta^*) = 0$, since, by periodicity $\pi = -\pi$. This violation of one of the original requirements amounts to a drastic multiplication of the number of Dirac particles: instead of one we end up with sixteen !

4 Overlap Dirac Operator

Any regularization deemphasizes the dynamics of short length/time scales. Lattice regularizations completely remove arbitrarily high momenta by compactifying momentum space. Thus, the spectrum of a lattice regularized Dirac operator lives on a compact space. When looking for a way around the chirality “no-go theorem” a possible line of attack is to prepare ahead of time for the regularization step by shifting the focus to an operator which already has a compact spectrum in the continuum.

Based on the anti-hermiticity of D_c (which we argued before can be viewed as a fundamental property, one that in conjunction with the other fundamental property of γ_5 -hermiticity produces chirality as a consequence) we can quite naturally define an associated unitary operator V_c using the Cayley transform:

$$V_c = \frac{D_c - A_c}{D_c + A_c} . \quad (11)$$

V_c is not only unitary, but also γ_5 -hermitian, inheriting the property from D_c . In other words, V_c has the two crucial properties of D_c and these two properties would imply chirality for D_c defined in terms of V_c by inverting

the Cayley transform (the inverse is another Cayley transform). Also, one has to note that the “no-go theorem” does not prohibit a lattice version of V_c , V , that satisfies both requirements of γ_5 -hermiticity and unitarity. However, the D one would construct from such a V would need to violate something - the natural choice is that D be non-local. Still, nothing seems to say that V itself has to be nonlocal:

$$D = \frac{1+V}{1-V} . \quad (12)$$

The non-locality in D , mandated by the “no-go theorem”, could reflect merely the existence of unit eigenvalues to V .

The next question is then, suppose we have a lattice V ; since D is non-local, how can we hope to make progress? The answer is almost trivial if we go back to continuum: we only care about the spectral part of D_c which is below some cutoff Λ_c . So, we are allowed to expand the Cayley transform:

$$V_c = -1 + 2\frac{D_c}{\Lambda_c} + O\left(\frac{D_c}{\Lambda_c}\right)^2 . \quad (13)$$

Therefore,

$$\frac{D_c}{\Lambda_c} = \frac{1+V_c}{2} \quad \text{plus unphysical corrections.} \quad (14)$$

If the lattice- V is local there is no locality problem with the lattice- D_o being given by

$$D_o = \frac{1+V}{2} . \quad (15)$$

Now, in agreement with the “no-go theorem”, we have lost exact anti-hermiticity, and, consequently exact, mathematical, chirality. However, the loss of chirality can be made inconsequential, unlike in the traditional Wilson formulation of fermions. As a first sign of this let us check that adding a mass term produces a lower bound similar to the continuum and thus would protect our precious condition number. It is easy to prove that:

$$\left(\frac{m_c}{\Lambda_c} + \frac{1+V_c}{2}\right)^\dagger \left(\frac{m_c}{\Lambda_c} + \frac{1+V_c}{2}\right) \geq \min \left[\left(\frac{m_c}{\Lambda_c}\right)^2, \left(\frac{m_c}{\Lambda_c} + 1\right)^2 \right] . \quad (16)$$

So, we have an expression bounded away from zero as long as $\frac{m_c}{\Lambda_c} \neq 0, -1$. Another way to see that we have as much chirality as we need is to calculate the anticommutator of D_o with γ_5 , which would be zero in the continuum, when D_c is used. Actually, in the language of path integrals, we do not really need the Dirac Operator itself: rather we need its inverse and its determinant. So, it is closer to physics to look at the inverse of the Overlap Dirac Operator D_o . D_o^{-1} obeys

$$\gamma_5 D_o^{-1} + D_o^{-1} \gamma_5 = 2\gamma_5 . \quad (17)$$

The same equation would also hold in the continuum if we replaced D_c^{-1} by $\frac{2}{1+V_c}$. There is little doubt that such a replacement in the continuum has no

physical consequence; after all it only changes D_c^{-1} additively, by -1 , a Dirac delta-function in space-time. While on the lattice we don't have a local and exactly chiral D , we do have a $D_o = \frac{1+V}{2}$ and we now see that *its* inverse is good enough. In a brilliant paper [4]⁶, published almost twenty years ago, Ginsparg and Wilson suggested this relaxation of the chirality condition as a way around the “no-go theorem”. What stopped progress was the failure of these authors to also produce an explicit formula for D_o . Their failure, apparently, was taken so seriously, that nobody tried to find an explicit D_o , and the entire idea fell into oblivion for an embarrassingly long time. Nobody even made the relatively straightforward observation that the search for D_o was algebraically equivalent to a search for a unitary, γ_5 -hermitian operator V . Moreover, it seems to have gone under-appreciated that the problem was not so much in satisfying the algebraic constraint of the relaxed form of the anticommutator (the GW relation), but, in simultaneously maintaining gauge covariance, discrete lattice symmetries, and correct low momentum behavior, without extra particles.

4.1 Definition and basic properties

To guess a lattice formula for V , first notice that, in the continuum, the operator $\epsilon_c = \gamma_5 V_c$ is a reflection: $\epsilon_c^2 = 1$ and $\epsilon_c^\dagger = \epsilon_c$. Also, V_c , and hence ϵ_c , are expressed as a ratio of *massive* Dirac operators. But, we know that there is no difficulty in representing on the lattice the massive Dirac Operator. The simplest way to do this is to use the Wilson Dirac Operator, D_W . The latter obeys γ_5 -hermiticity, so $H_W = \gamma_5 D_W$ is hermitian. It is then very natural to try

$$\epsilon = \text{sign}(H_W) . \quad (18)$$

This is not the entire story - we still have one parameter at our disposal, the lattice mass, m . When we look at the continuum definition of V_c we observe that it can be rewritten as follows:

$$V_c = \frac{D_c - \Lambda_c}{\sqrt{-D_c^2 + \Lambda_c^2}} \frac{\sqrt{-D_c^2 + \Lambda_c^2}}{D_c + \Lambda_c} . \quad (19)$$

So V_c is given by the product of two unitary operators, one being the unitary factor of the Dirac Operator with a large negative mass and the other the conjugate of the unitary factor of the Dirac Operator with a large positive mass. Formally, the unitary factors are equal to each other up to sign in the

⁶ Clearly, when going to the lattice, the continuum delta-function can be replaced by a Kroneker delta-function or by, say, a narrow Gaussian. This gives a certain amount of freedom which I shall ignore below. In the lattice formulation of Ginsparg and Wilson this freedom is made explicit by the introduction of a local operator R .

continuum and one has:

$$V_c = -U_c^2 = -\left(\frac{D_c - A_c}{\sqrt{-D_c^2 + A_c^2}}\right)^2; \quad -D_c^2 + A_c^2 = (D_c - A_c)^\dagger (D_c - A_c) . \quad (20)$$

But, on the lattice, a local unitary operator U replacing U_c cannot exist; if it did, $D = \frac{1}{2}(U^\dagger - U)$ would violate the “no-go theorem”. So, on the lattice we can find a V , but there is no local square root of $-V$; this observation is rather deep, and related to anomalies. We need to treat the two unitary factors in the continuum expression for V_c differently on the lattice. Actually, the factor with a positive mass sign can be replaced by unity by taking the limit $m \rightarrow \infty$, something one can do only on the lattice, where the T_μ operators are bounded. The factor representing negative mass however cannot be so simplified because the negative mass argument m is restricted to a finite interval ($-2 < m < 0$) to avoid extra particles. Thus, on the lattice we are led to

$$V = D_W(m) \frac{1}{\sqrt{D_W^\dagger(m) D_W(m)}} \quad \text{with} \quad -2 < m < 0 . \quad (21)$$

This formula is equivalent to the one for ϵ above. The reason that we get exactly massless quarks is that no fine tuning is needed for V to have eigenvalues very close to -1 . Indeed, $D_W(m) = D_W(0) + m$ and, in the case $[T_\mu, T_\nu] = 0$, $D_W(0)$ is easily seen to have very small eigenvalues. There $D_W(m)$ is dominated by the negative mass m . It is unimportant what the exact value of m is, only its sign matters. Even when $[T_\mu, T_\nu] \neq 0$, and m is additively renormalized, as long as the effective m stays negative, we shall have exactly massless quarks as evidenced by the eigenvalues of V close to -1 potentially producing long range correlations in D_o^{-1} .

All non-real eigenvalues of V are paired: $V\psi = e^{iv}\psi \Rightarrow V\gamma_5\psi = e^{-iv}\gamma_5\psi$. But, one important property of the continuum V_c is that it has an unpaired single -1 eigenvalue in a certain class of topologically nontrivial backgrounds. This is a characteristic of massless quarks and has to be reproduced on the lattice. There V is even dimensional, so a single exact $V = -1$ state implies the existence of another $V = +1$ state. In addition, it is clear that as a result of $|m| < 2$, there are states where $D_W(0)$ dominates over m and these states will have eigenvalues far off the real axis. We conclude that the spectrum of V can cover the entire complex unit circle. The spectrum of U_c though, covers only half the complex unit circle. This is a reflection of V being a lattice version of $-U_c^2$ rather than U_c itself, as one might think naively.

It was mentioned already that all one needs in the path integral are formulae for the inverse of the Dirac Operator and for its determinant. It is clear that once one has an acceptable V one can form not only the local, but not strictly chiral operator D_o but also a non-local chiral associate $D_o^\chi = \frac{1+V}{1-V}$. In the determinant one must use D_o and cannot use D_o^χ . Otherwise, the extra

zeros of the determinant coming from the $V = 1$ states leave an indelible effect in the continuum limit. These zeros directly reflect the non-locality of D_o^χ . However, the inverses of D_o can be replaced by inverses of D_o^χ which has useful practical implications. In the language of Feynman graphs, the determinant is represented by closed internal fermion loops, and on those we must use D_o^{-1} , but the inverses come from external fermions lines, and on those we can just as well use $D_o^{\chi-1} = D_o^{-1} - 1$. This is consistent because the -1 term can be interpreted as coming from an auxiliary fermionic variable which contributes only a unit multiplicative factor to the fermionic determinant.

To complete the logic of the story let me discuss the introduction of a finite quark mass parameter in the context of the Overlap Dirac Operator. To be sure there is no additive mass renormalization, one wishes to preserve the continuum property that $Tr \frac{1}{D_c + m_c}$ is odd in m_c ; this property⁷ singles out the point $m_c = 0$. This property is a direct consequence of $\gamma_5 D_c + D_c \gamma_5 = 0$. It is easy to see that for an external fermion line the lattice version would be

$$Tr \frac{e^\rho - V}{e^\rho + V} = Tr \left(\frac{2}{1 + e^{-\rho} V} - 1 \right); \quad \rho > 0; \quad (22)$$

with

$$m_q = z \tanh \frac{\rho}{2}; \quad \left(\frac{1 + V}{2} \right)_{T_\mu = \exp(i\theta_\mu)} \longrightarrow \frac{i}{z} \sum_\mu \gamma_\mu \theta_\mu + O(\theta_\mu^2) . \quad (23)$$

The factor z is somewhere between 1 and 2. One now easily proves that the condition number of the matrix $\frac{e^\rho + V}{e^\rho - V}$ is $\frac{1}{\tanh(\frac{\rho}{2})} = \frac{z}{m_q}$. Therefore, we should be able to get to the quark masses we need. However, the matrix ϵ isn't sparse, and the evaluation of its action will be time consuming. Still, it is a function of a sparse matrix H_W , so employing the Overlap Dirac Operator in numerical QCD is not ruled out *ab initio*.

4.2 Implementation by rational approximants

The operator ϵ is unambiguously defined only for matrices H_W that have no zero eigenvalues. This is not a restriction in itself, because the variables $U_\mu(x)$ in H_W are stochastic and there is no symmetry protecting zero eigenvalues of H_W . So, the probability to encounter an exact zero of H_W is zero. Moreover, in the continuum limit H_W will have a relatively large gap around zero, so when we are close enough to the continuum we need the sign function only over the range of arguments $[-a, -b] \cup [b, a]$, where $a \sim 8$ and b should be something like 0.1 or 0.5.

Over the above range it is relatively easy to approximate the sign function by simpler functions. Also, for b uniformly (in the background) bounded away

⁷ A less careful introduction of non-zero quark mass in the Overlap Dirac Operator requires extra unnecessary subtractions - see [6].

from zero, the operator $\frac{1}{\sqrt{D_W^\dagger D_W}}$ is a convergent series in H_W . This ensures that the non-sparse D_o is nevertheless sufficiently local to be an acceptable approximation to a continuum differential operator.

Mimicking the way transcendental functions are typically implemented in computers, we are led to try a rational approximation [7]. So, we are looking for a series of functions $\varepsilon_n(x)$ which, for any fixed $x \neq 0$, obeys $\lim_{n \rightarrow \infty} \varepsilon_n(x) = \text{sign}(x)$. For each finite n , $\varepsilon_n(x)$ is a ratio of two polynomials. A sequence with many good properties has been in use by applied mathematicians [5] who were interested in the sign function because of the role it plays in control theory. The sequence is given by:

$$\varepsilon_n(x) = \frac{(1+x)^{2n} - (1-x)^{2n}}{(1+x)^{2n} + (1-x)^{2n}} = \begin{cases} |x| < 1 & \tanh[2n \tanh^{-1}(x)] \\ |x| > 1 & \tanh[2n \tanh^{-1}(x^{-1})] \\ |x| = 1 & x \end{cases} \quad (24)$$

So long $|x|$ is sufficiently far from zero a large enough n can provide an approximation to the sign function good to machine accuracy. The approximants $\varepsilon_n(x)$ are smooth and maintain some properties of the sign function:

$$\varepsilon_n(x) = -\varepsilon_n(-x) = \varepsilon_n\left(\frac{1}{x}\right); \quad |\varepsilon_n(x)| \leq 1; \quad \varepsilon_n(\pm 1) = \pm 1. \quad (25)$$

To implement $\varepsilon_n(x)$ we decompose $f(x^2) = \varepsilon_n(x)/x$ in simple pole terms:

$$\varepsilon_n(x) = \frac{x}{n} \sum_{s=1}^n \frac{1}{x^2 \cos^2 \frac{\pi}{2n}(s - \frac{1}{2}) + \sin^2 \frac{\pi}{2n}(s - \frac{1}{2})}. \quad (26)$$

One can choose an appropriate scaling parameter $\lambda > 0$ and approximate the sign function of H_W by $\varepsilon_n(\lambda H_W)$. The action of this approximated ε on a vector ψ can be evaluated by a multi-shift Conjugate Gradient inversion algorithm [8]. The multi-shift trick reduces the computational cost of evaluating the action of each one of the terms in the pole expansion to the cost of evaluating one single inversion, the most time consuming one, which clearly is

$$\frac{1}{\lambda^2 H_W^2 + \tan^2 \frac{\pi}{4n}} \psi. \quad (27)$$

Memory requirements are linear in n , since one needs to store a few vectors for each pole term. In practice this may be a problem, not as much that the entire memory of the machine would be exceeded, but rather that one would find oneself exceeding the level 2 cache. Level 2 cache misses can lead to substantial performance loss. Thus, it is useful to consider an alternative to the standard implementation of the multi-shift trick. Usually, in applications of the multi-shift trick, one is really interested in the individual vectors, but here we only want their weighted sum. It is quite easy to figure out a way to store only a few vectors, and get the sum, but a double pass over the basic Conjugate Gradient procedure is now required. Although the number of

floating point operations is doubled, because of reduced cache miss penalties, performance is not necessarily adversely impacted and can actually increase [9].

Other promising methods to implement D_o have been developed and will be hopefully discussed here later [10]. In the implementation employed in [6] the sign function was approximated by a very high order polynomial.

4.3 A new bottleneck and projectors

Having removed one apparent obstacle, namely the potentially large memory requirements, we turn to a much more substantial obstacle, namely the condition number of H_W^2 , κ . κ determines both the number of Conjugate Gradient iterations needed to evaluate the inverse and also the minimal required n for given expected accuracy δ , where

$$\|\varepsilon_n(\lambda H_W) - \text{sign}(H_W)\| < \delta . \quad (28)$$

The optimal choice of λ is easily found because of the inversion symmetry of $\varepsilon_n(x)$: $\lambda h_{\min} = \frac{1}{\lambda h_{\max}}$ where $h_{\min, \max}$ are the square roots of the minimal and maximal eigenvalues of H_W^2 . Thus, $\lambda = \frac{1}{\sqrt{h_{\min} h_{\max}}}$ so the range over which the sign function is needed is

$$\frac{1}{\kappa^{\frac{1}{4}}} < |x| < \kappa^{\frac{1}{4}} . \quad (29)$$

For $\varepsilon_n(x)$ to be an acceptable approximation we need then $n \approx \frac{1}{4} \kappa^{\frac{1}{4}} |\log(\delta/2)|$. For example, for $\kappa \sim 10^4$ and single precision $n \sim 50$ is safe; for double precision, the needed n doubles. On the other hand the number of Conjugate Gradient iterations will go as $\kappa^{\frac{1}{2}}$. Note that the lowest eigenvalue of $\lambda^2 H_W^2$ and the minimal pole shift $\frac{\pi^2}{16n^2}$ are of the same order when $n \sim \kappa^{\frac{1}{4}}$.

Comparing to traditional simulations, where κ is again the source of all problems, it is important to note the new feature that now the parameter m in H_W is taken in a different regime from before. In traditional simulations the parameter m is adjusted so that the physical quark mass be small. This precisely means that the parameter is chosen so that κ be large. Because of fluctuations, κ becomes often much larger than one would have expected, and that is the problem faced by traditional simulations discussed earlier. Here the parameter m , subject to the limitation $-2 < m < 0$, can be chosen so that κ be as small as possible. Fluctuations can still cause problems and sometimes make κ large, but, in principle, the fluctuations are around a small κ value, not a large one. In practice however the situation is somewhat marginal: coarse lattices produce too much fluctuations even for the Overlap Dirac Operator. But, finer lattices are manageable. Still, even on finer lattices one needs to split the domain over which the sign function is approximated into a neighborhood around zero and the rest. The neighborhood around zero

contains of the order of ten eigenvalues, and by computing the exact projector on the corresponding eigenspace, the sign function is exactly evaluated there, leaving only the more manageable part of the spectrum to be dealt with by the rational approximation [11]. This is quite time consuming, and constitutes the new bottleneck we are facing. Variations of the probability distribution of the background and slight modifications of H_W would not affect the continuum limit but would probably help ameliorate this problem.

4.4 Avoiding nested Conjugate Gradient procedures

Another obvious drawback of using the Overlap Dirac Operator in numerical simulations is that we eventually need to compute vectors of the form $\frac{2}{1+V}\psi$ for a given ψ . This requires another inversion and we end up with a two level nested Conjugate Gradient procedure, whereas in the traditional simulations we only had one. The outer Conjugate Gradient is going to be better conditioned (for light but still massive quarks) than in the traditional approach. So, we are facing a tradeoff issue, one that has not been resolved yet. The two levels of Conjugate Gradients are presently dealt with separately, but clearly, eventually, potential gains will be obtained from the fact that the inner procedure does not have to be run to high accuracy for the initial steps in the outer procedure.

There exists another trick [12] to simulate the rational $\varepsilon_n(\lambda H_W)$ which does away with the need of employing a nested conjugate gradient altogether, but at the expense of memory usage linear in n . Basically, the point is to find a Conjugate Gradient algorithm operating in an enlarged space and producing the vector $\frac{2}{1+V}\psi$ in one blow. This trick is based on two observations:

1. Any rational approximation can be written as a truncated continued fraction.
2. Any truncated continued fraction can be represented by a Gaussian Path Integral of a fermionic system living on a chain of length n , where n is the depth of the truncated continued fraction.

This method is applicable to any rational approximation. Below is one way to apply it to $\varepsilon_n(H_W)$, where the scale factor is absorbed in H_W for notational simplicity.

First, the rational approximation has to be written in the form of a continued fraction with entries preferably linear in H_W . I start from a formula that goes as far back as Euler, and subsequently use the invariance under inversion of x to move the x factors around, so that the entries become linear

in x .

$$\varepsilon_n(x) = \frac{2nx}{1 + \frac{(4n^2 - 1)x^2}{3 + \frac{(4n^2 - 4)x^2}{5 + \dots \frac{\ddots}{4n - 3 + \frac{[4n^2 - (2n - 1)^2]x^2}{4n - 1}}}}} \quad (30)$$

Now, with the help of extra fields, I write a Gaussian path integral which induces the desired action between a chosen subset of fields:

$$\int d\bar{\phi}_1 d\phi_1 d\bar{\phi}_2 d\phi_2 \dots d\bar{\phi}_n d\phi_n e^{S_*} = (\det H_W)^{2n} e^{-\bar{\psi}(\gamma_5 + \varepsilon_n(H_W))\psi} . \quad (31)$$

The quadratic action S_* couples the extended fermionic fields $\bar{\chi}, \chi$:

$$\bar{\chi} = (\bar{\psi} \quad \bar{\phi}_1 \quad \dots \quad \bar{\phi}_{2n}), \quad \chi = \begin{pmatrix} \psi \\ \phi_1 \\ \vdots \\ \phi_{2n} \end{pmatrix} . \quad (32)$$

$S_* = \bar{\chi} \mathbf{H} \chi$, where the new kernel, \mathbf{H} , has the following block structure:

$$\mathbf{H} = \begin{pmatrix} -\gamma_5 & \sqrt{\alpha_0} & 0 & \dots & \dots & 0 \\ \sqrt{\alpha_0} & H_W & \sqrt{\alpha_1} & \dots & \dots & 0 \\ 0 & \sqrt{\alpha_1} & -H_W & \dots & \dots & 0 \\ \dots & \dots & \dots & \ddots & \dots & 0 \\ \dots & \dots & \dots & \dots & H_W & \sqrt{\alpha_{2n-1}} \\ \dots & \dots & \dots & \dots & \sqrt{\alpha_{2n-1}} & -H_W \end{pmatrix} \quad (33)$$

The numerical coefficients α are given below:

$$\alpha_0 = 2n, \quad \alpha_j = \frac{(2n - j)(2n + j)}{(2j - 1)(2j + 1)}, \quad j = 1, 2, \dots \quad (34)$$

The hope is that the condition number of \mathbf{H} will be manageable. The basic point is that up to a scalar factor, the (1,1) diagonal block of the inverse \mathbf{H}^{-1} is equal to $\frac{1}{1+V}\gamma_5$. \mathbf{H} is sparse and the evaluation of $\mathbf{H}^{-1}\chi$ requires one single Conjugate Gradient procedure, albeit one acting on vectors $2n$ times longer than needed. Although I used Path Integrals to get the relation between \mathbf{H} and the Overlap Dirac Operator, there is nothing more to the derivation than ordinary Linear Algebra, and Path Integrals could have been bypassed altogether.

So, at the expense of adding extra fields one can avoid a nested Conjugate Gradient procedure. This would be particularly important when dynamical

fermions are simulated. The chain version of the direct truncation of the Overlap Dirac Operator is similar in appearance to another truncation, usually referred to as “domain walls” [13].

The proposal above, employing chains, has two potential advantages over domain walls. First, it is much more flexible, allowing one to change both the rational approximation one uses and its chain implementation. This flexibility ought to allow various improvements. Second, since here the argument of the approximated sign function is λH_W , not the rather cumbersome logarithm of the transfer matrix of the domain wall case, eigenstates of H_W with small eigenvalues can be eliminated by projection with greater ease. This elimination, although costly numerically, vastly increases the accuracy of the approximation to the sign function. Actually, at this stage of the game and at practical gauge coupling values, the use of projectors seems to be numerically indispensable to direct implementations of the Overlap Dirac Operator. Although no projectors have been implemented in domain wall simulations and physical results have been claimed, to me it seems doubtful that the domain wall version of truncating the Overlap will really be capable to get to small quark masses without employing some technique equivalent to projection.

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